Program documentation of the ViPErLEED ImageJ plugins

For version V1.02 of the plugin set

Updated version of the Supplemental Material for the paper

ViPErLEED package II: Spot tracking, extraction, and processing of *I*(*V*) curves

Michael Schmid,[1] Florian Kraushofer,[1,2] Alexander M. Imre,[1] Tilman Kißlinger,[3] Lutz Hammer,[3] Ulrike Diebold,[1] and Michele Riva[1]

[1] *Institute of Applied Physics, TU Wien, Vienna, Austria*
[2] *Department of Chemistry, TUM School of Natural Sciences, Technical University of Munich, Garching bei München, Germany*
[3] *Solid State Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany*

Phys. Rev. Research 7, 013006 (2025)

Contents

Installation

ImageJ can be downloaded from https://imagej.net/ij/download.html.* After installation, the program should be updated to the latest version with *Help>Update ImageJ…* (from inside the ImageJ program). This replaces the `ij.jar` file in the ImageJ directory with the latest version and requires that the user has write access to the ImageJ directory. If *Help>Update ImageJ* did not work, take the `ij.jar` file from http://wsr.imagej.net/download/daily-build/ and place it in the ImageJ directory (replace the old one). On MacIntosh OS X, you have to right-click the ImageJ icon and select "Show Package Contents". The `ij.jar` file is in `Contents/Resources/Java`.

Make sure that ImageJ has enough memory (≈10 GB recommended, but not more than 70% of total RAM). Memory is assigned in the *Edit>Options>Memory&Threads* menu, then restart ImageJ.

The ViPErLEED plugins are available at https://github.com/viperleed/viperleed-imagej and contained in the file `ViPErLEED_ImageJ_plugins.jar`. The most recent version can be downloaded under https://github.com/viperleed/viperleed-imagej/releases/latest. This Java archive should be placed into ImageJ/plugins or a subdirectory thereof. After restarting ImageJ, a menu entry *Plugins>ViPErLEED* will appear.

Notes for Developers

The file `ViPErLEED_ImageJ_plugins.jar` is a zip archive and contains the compiled Java `.class` files, a file `plugins.config`, which determines which commands appear in the ImageJ menus and where. The `ViPErLEED_ImageJ_plugins.jar` file also contains the source code. The source code is also available at https://github.com/viperleed/viperleed-imagej.

If you want to modify the plugins, place the source files into a subdirectory of ImageJ/plugins. To avoid version conflicts, move the `ViPErLEED_ImageJ_plugins.jar` to a place outside ImageJ/plugins (alternatively, rename it such that it becomes inactive, i.e., the extension must not be .jar or .zip), and restart ImageJ. Now the sources can be compiled from within ImageJ with *Plugins>Compile & Run…* and used essentially the same way as previously the files in `ViPErLEED_ImageJ_plugins.jar`. After *Help>Refresh Menus* or restarting ImageJ, the compiled plugins will appear in the *Plugins* menu of ImageJ, under a submenu entry with the name of the directory where they reside. Note that the command *Plugins>Compile & Run…* currently does not work with the Fiji distribution of ImageJ; users of Fiji have to use the script editor, available via *File>New>Script*, open the java file and compile with "Run".

The main classes that are accessible from the ImageJ *Plugins* menu should have an underscore in the name; others are auxiliary classes; these are automatically compiled with the main class. To avoid conflicts with other plugins, all classes in the ViPErLEED package contain `LEED_` or `Leed` in the name (the latter for auxiliary classes that are not a plugin).

---

* On macOS 15, after installing ImageJ, the following steps may be required (in a terminal window):
`cd` to the directory containing your ImageJ.app. Then type

```
sudo chflags -R nouchg ImageJ.app
sudo xattr -rd com.apple.quarantine ImageJ.app
```

When modifying the sources and compiling, note that the ImageJ compiler currently only checks for updates of the plugin class compiled and classes directly called from the plugin class; it does not recognize modifications of an auxiliary class that is called only from another auxiliary class. In such a case, either delete the `.class` file of the modified auxiliary class after modification of its `.java` file, or compile the auxiliary `.java` file separately, or declare a dummy variable with the uncalled auxiliary class in the plugin, to enforce checking for modifications of the sources of this class.

If the newly compiled version works as desired, you can replace the `.class` files in `ViPErLEED_ImageJ_plugins.jar` with the new version, make this `.jar` active again (move it back to ImageJ/plugins or rename it back), and delete the individual `.class` files in your subdirectory of ImageJ/plugins. Then restart ImageJ. When the class files are contained in `ViPErLEED_ImageJ_plugins.jar`, the plugins.config file contained in the `.jar` determines which commands appear in the ImageJ menus and where.

Notes on the documentation

Almost all of the documentation text in the following is a copy of the program help, which can be accessed via the Help buttons, augmented by several screen shots. You can copy the contents of any help window (CTRL-a to select all and CTRL-c[1]). Paste it into a text editor for printing, annotating, etc.

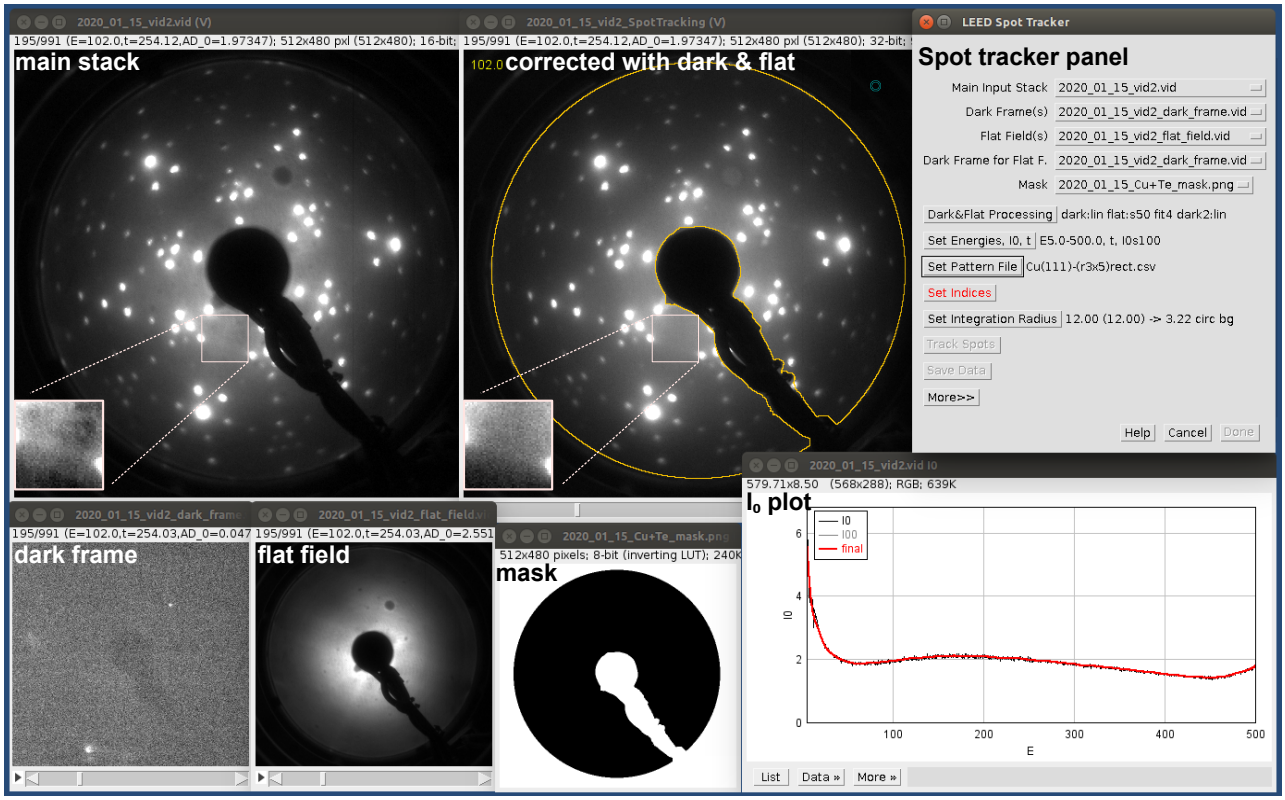
Updates of this documentation will be published at https://www.viperleed.org/

License

When using this program (in its original or modified form) for scientific work, please cite the paper describing the program [1].

ViPErLEED Spot Tracker

This ImageJ plugin is used to extract intensity vs. energy curves [a.k.a. $I(V)$ curves] from low-energy electron diffraction (LEED) movies.



Input Images/Stacks

Main Input Stack (required)

The movie with the LEED images (must have evenly spaced electron energies, unless intensity vs. time or some other data channel at constant energy should be measured).

Dark Frame and Flat Field (optional)

These images should be used to correct for the dark current of the camera (and background illumination, if any) as well as inhomogeneities of the LEED screen, optics, and camera. The *flat field* is an image (or image stack) of a diffuse diffraction pattern with no spots, only showing the inhomogeneities of the optics and camera. The flat field is typically recorded by moving a polycrystalline sample holder to the sample position; make sure that the distance from the electron source is exactly the same as that of the sample surface. (Since the intensity is spread out over all the screen, you may use a higher beam current or longer exposure than for the LEED movie of the sample.) A flat field is especially important if the LEED image has a high background intensity, e.g., for sample temperatures around or above the Debye temperature of the sample. *Dark frame* images (when present) are subtracted from the input stack and flat field before the flat-field correction. The dark frame is best measured with a high negative Wehnelt voltage, suppressing the beam, but keeping light emitted by the filament as well as any glow due to (field-emitted) electrons reaching the

fluorescent screen.
The formula is

```
corrected_pixel_value = (input - dark)/(flat - dark2)
```

where `dark2` is the dark frame for the flat field (usually the same as the dark frame of the main input, unless the main input and flat field differ in the exposure time or gain). If a dark frame is not given, nothing is subtracted there.

The `(flat - dark2)` values must be positive in the area defined by the mask (see below). In case of negative or zero values (e.g., due to excessive noise), attempts to track (and measure) the LEED spots will result in an error message.

For the dark and flat images, one can provide a stack. If the stack has the same number of images as the main input, it is used image-by-image for the corresponding main input image. There is no check whether the energies are the same as for the main stack; this is your responsibility. Preprocessing of these correction image stacks (e.g., averaging over a few energies to reduce noise, 2D fitting or at least intensity normalization for the flat field) should be selected with *Dark & Flat Processing*. If the number of images of a dark or flat stack differs from that of the main input stack, they are averaged and this average is used for all images of the main input. (If the `flat` is a single image or an average, the `dark2` also uses the average over the stack, even if it has the same number of images as the main input.) The type of dark & flat processing is displayed in abbreviated form next to the *Dark & Flat Processing* button. Some sort of averaging (to reduce the noise) is advisable, especially for the flat field.

Note that image processing with dark and flat requires a *mask* (see below). The mask defines the area where the correction will be performed. Without a proper mask, the correction will result in arbitrary values outside the LEED screen; this will prevent proper setting of brightness & contrast and may make the LEED screen appear black or dull.

Mask (required)

An 8-bit image ("binary image") with white pixels for the background and black for the foreground. The foreground area determines the screen area where intensities may be measured. The mask image must NOT contain pixel values other than 0 or 255. You can use *Analyze>Histogram* to see which pixel values are present in an image; in the histogram panel click on "Log" (logarithmic *y* axis scale) to see also values that occur for a few pixels only. You can use *Image>Adjust>Threshold* (and "Apply") to ensure that all pixel values are 0 or 255. Images with in-between values cannot be selected as a mask.

You have to create the Mask image; start with *More>>Create Mask*. As soon as a mask has been created and selected, it is shown as an outline on the image stack used for spot tracking. Editing of the mask image will be reflected by the outline almost immediately.

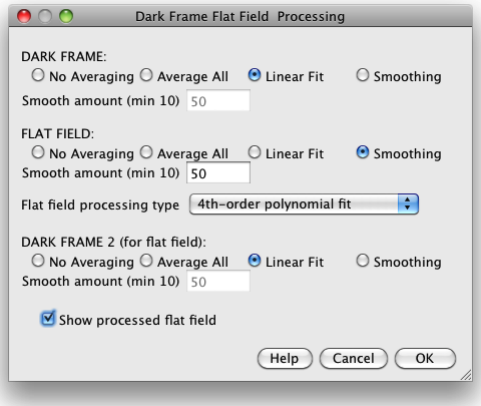
All these images or image stacks must be open in ImageJ; you can use *More>>Open Images/Movies…* on the spot tracker to open them (and select them as the input, if appropriate). Alternatively, you can use the *Plugins>ViPErLEED>Open LEED Movie...* command (which can also create a table of metadata when opening a movie) or the various ImageJ *File>Open* and *File>Import* commands (e.g. *File>Import>Image Sequence…*) for combining multiple images into an image stack (i.e., a movie). Image stacks may be in

memory or (if the open/import command allows) they can be *virtual stacks*, i.e., the active image is read from disk as required, but not always kept in memory (needs less RAM).

All these images or stacks must have the same width and height (in pixels). Do not close these images or stacks while using the ViPErLEED Spot Tracker.

Dark & Flat Processing

If the dark frame and flat field (and the dark2; this is the dark frame subtracted from the flat field) are stacks with the same number of slices as the main input stack, one can select several options:
- No averaging: The correction images should be applied slice by slice. In this case, any noise of the correction images will increase the noise of the result.
- Average all: Best noise suppression, but no energy dependence (usually not suitable for the flat field).
- Linear fit: This provides good noise suppression, but keeps linear drift with energy or time. This option can be useful especially for the dark frames.
- Smoothing: Select this option for averaging over a few energies (usually used for the flat field). The *Smooth amount* determines the noise suppression. (For a smooth amount of *n*, the noise suppression is roughly equivalent to that of averaging over *n* stack slices, but the algorithm is actually different from moving averages, with better suppression of rapid fluctuations and less memory use.)



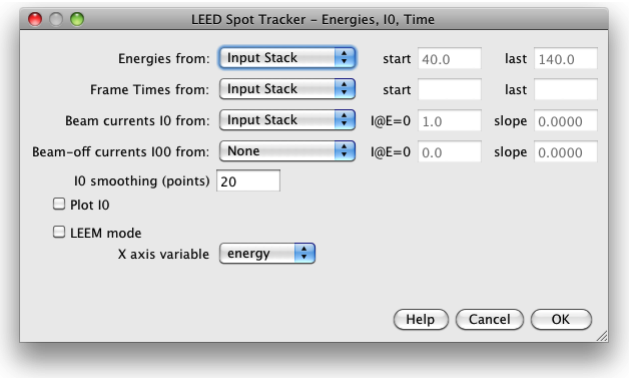
Flat field processing type: Before applying the flat field (and after subtraction of its dark frame, if provided) to the main image, in most cases further processing of the flat field should be applied: If the flat field is a stack with 1:1 correspondence to the input (i.e., same number of slices), one should select at least normalization, i.e., keeping the average intensity of the stack (across the mask area) constant. Furthermore, usually the flat-field intensity decreases towards the edge, because diffuse scattering intensity from a polycrystalline sample tends to peak at a scattering angle of 180° (backscattering). Then one should correct the (background-corrected) flat field by a fit of a 2nd-order or 4th-order polynomial to its logarithm (for 2nd-order, this would approximately correspond to division by a best-fit Gaussian; the 4th-order fit is usually preferable, but slower to compute). Polynomial fits should be only applied if the long-range intensity variations of the flat field are due to the scattering process in obtaining the flat field, not if these variations are due inhomogeneous efficiency of the LEED screen or vignetting of the camera.

One can examine the flat field (after all processing steps) by *Show processed flat field*. The output of *Show processed flat field* can be also used for further processing of the flat field by any image processing method of your choice, then the result of this processing can be used as a flat field further on. In this case do not forget to deselect the dark frame for the flat field and deactivate the polynomial fit (unless you really want it).

Note that processing steps that require all images of an input stack, such as averaging over all images or a linear fit over all images of a stack require some computing time. It may take several seconds until the processed result becomes available; this may also cause a delay in opening the Spot Tracker main panel

when it automatically selects the input images or stacks. Expect delays especially if the inputs are supplied as virtual stacks (i.e., not kept in memory but read from disk on demand).

Set Energies, I0, t



The energy range of the input stack, the beam current I0 (for normalization), and the time (with respect to the first slice) are usually read from the slice labels of the main input stack; they are read in when reading the main image stack. If these data were not available, one can set them manually, as a linear function or from a table that has been opened by ImageJ. [Note that one can open `.csv` and `.tsv` files (comma- or tab-separated values)[2] as tables with ImageJ, if they contain exactly one header line.] The "Set Energies, I0, t" dialog also provides an entry for I00, the offset of the beam current I0. I00 can be also read from the I0 values of the dark frame(s) (if present), either using the individual values for each energy or a linear fit (if the dark frames are a stack with 1:1 correspondence to the main input stack). I00 may be read from the dark frame(s) only if they were obtained without emitted electron current (i.e., by setting the Wehnelt voltage to a highly negative value, not by setting the screen voltage to 0). If I00 is provided, the actual beam current is calculated as `I0 - I00`. Usually, the beam current should be smoothed; the amount of smoothing can be entered (0 for no smoothing). The amount of smoothing is given as the number of points in a moving-averages filter with the same noise suppression; actually a modified sinc kernel [2] is used. I0, I00, and the smoothed and I00-corrected beam current are plotted after closing this input window if 'Plot I0' is selected. The plot does not include corrections based on the background intensity measured during spot tracking (after spot tracking, you can use *More>>Plot...* for this).

This input window also has an option to set LEEM mode. In LEEM mode, it is assumed that the spots do not move with energy as they would in normal LEED experiments.

For experiments with constant electron energy, such as studies of phase transitions (over temperature) or evolution over time, one can specify an *x* axis other than the energy.

In the Spot Tracker panel, the data present are indicated to the right of the 'Set Energies, I0, t' button; the sources of these data are given in square brackets (if not the input stack): `[T]` table, `[!]` manual input of a linear relationship, `[?]` kept previous data. For I00, `[D]` indicates values from the dark frames (lowercase `[d]` if I00 is a linear fit).

Set Pattern File

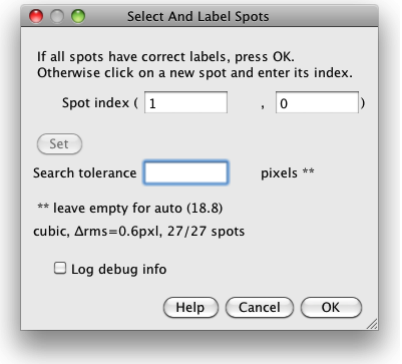
This file describes which beams (spots) are expected and their relative positions in a Cartesian coordinate system. This is a comma-separated (csv) file, one line for each diffraction maximum (beam), with the beam label, beam h and k indices, Cartesian reciprocal-space coordinates g_x, g_y, and a beam group index (same for equivalent beams). Such a file can be created with the pattern simulator of the ViPErLEED GUI (there, use Export from the File Menu). For creating the Spot pattern file in the ViPErLEED GUI, instead of manually

entering the symmetry, you can also read the symmetry from the `experiment-symmetry.ini` file created when running a LEED *I*(*V*) simulation with `viperleed.calc`.

Set Indices

Firstly, an input window appears and asks you to select a stack slice [an energy in usual *I*(*V*) measurements] where as many spots as possible are clearly visible, including spots near the edge of the screen. Use the slider below the '`...SpotTracking`' image stack to select the energy. (For energy selection, you cannot use one of the image stacks supplied as the input, unless it is coupled with the '`...SpotTracking`' stack via *Analyze>Tools>Synchronize Windows*). You may use the `Auto` button of the *Image>Adjust>Brightness&Contrast* panel (B&C; keyboard shortcut CTRL-SHIFT-C[1] when the stack is in the foreground) or the sliders of the B&C panel to adjust the contrast. If many spots are not recognized (not marked by a circle), or many circles do not mark diffraction maxima, you can adjust the noise rejection. Note that also an improper value of the integration radius may prevent recognition of the spots. Having a few 'false' spots marked does not hurt as long as these are not close to the position where a diffraction maximum would be expected.

When spot indices have been defined previously and fit the maxima, the maxima will be labeled and you can click 'Labels are OK' if the identification is correct. Otherwise, you have to manually name one or a few spots in the next step.



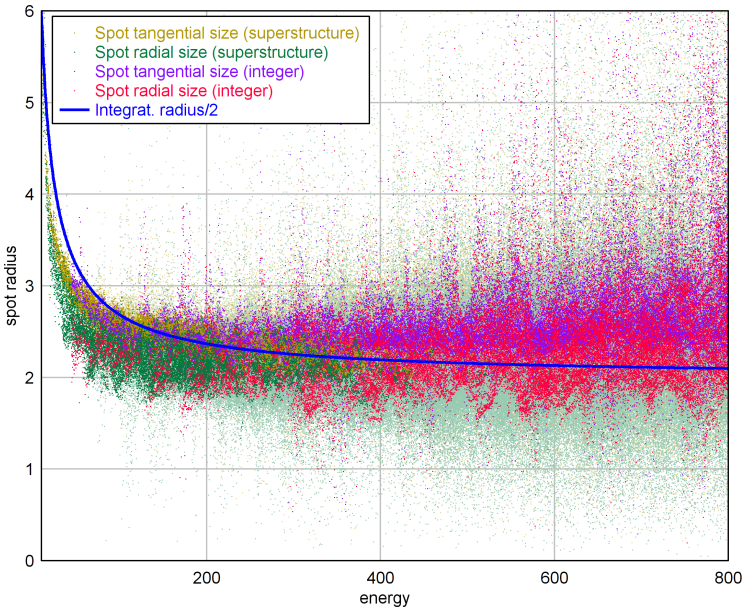
For naming the spots, a second input window asks you to select a spot by clicking on it and enter its h, k indices (for superstructures, also fractions are allowed). The spot must be listed in the pattern file. After pressing *Set*, the program tries to name the other spots. Examine the outcome (you may select the image and press '+' or CTRL-'+'[1] to zoom in at the cursor position). If the spots are named correctly, press OK; otherwise select another spot and enter its designation (best, choose a spot that has not been correctly identified). For LEED patterns recorded with oblique incidence (> 10° off-normal) it will be necessary to enter several spots. In that case, start with naming a few nearby spots. In case of a mistake, you can click on a spot and rename it. As soon as the program has tried to identify the spot pattern, the input window also shows the polynomial order it uses to convert reciprocal-space coordinates to pixel coordinates and the root-mean-square (rms) deviation of the spots from the fit in pixels. For small images (e.g., 512 × 512 pixels), the rms deviation should not be much more than about two pixels; otherwise carefully check whether the assignment is correct (especially if spots are dense in some places, but with larger gaps in between, as it happens for some superstructure cells). Especially in case of distorted images, one can also try to adjust the search tolerance (larger values allow for more distortions, but are more likely to result in incorrect spot assignment).

Set Integration Radius

The integration radius should be selected such that the spots are fully enclosed by a circle with the given radius. For low energies, where additional broadening due finite domain and terrace sizes (as well as the

electron source) may occur, the integration radius can be given separately for integer and superstructure spots.

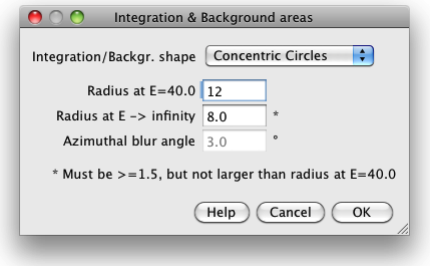
The output after spot tracking contains a plot with the measured spot radii and a line with half the integration radius as a function of energy. The point cloud should be mostly below the line. If there is no danger of the background area (see below) overlapping with neighboring spots, and noise is low, set an integration radius about 2.5 times the spot radii measured during spot tracking. (Then the line in the plot should be at ~1.2 times the typical values of the point cloud.) Large integration radii lead to lower noise for strong spots, but poorer performance for weak ones (more noise and more errors in case of an uneven background). One may use up to 3 times the typical spot radii if (i) the noise of the images is very low, and (ii) the background due to inelastic scattering is very low and flat, and (iii) all spots are bright. Even in case of very close spots and high noise, the radius values should not be less than ~2 times the typical spot radii. This means that the line in the spot radii plot should still be above the center of the point cloud. Usually it is a good idea to try spot tracking with different radii and compare the *I*(*V*) quality plots to find out which value works best. Keep in mind that the radii must be chosen such that the background area of each spot does not overlap with any of the neighboring spots.



Example of a Spot Radii plot created when tracking the spots.

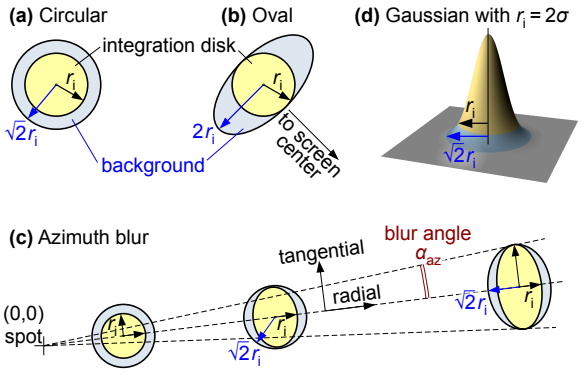
The spot radius was set to 12 pixels at the lowest energy (10 eV) and 4 pixels at E → ∞. At low energies, the point cloud is below the blue line; one might therefore use a smaller radius at E = 10 eV. At high energies, the center of the point cloud is above the blue line; it is therefore recommended to slightly increase the radius (e.g., to 5 pixels).

Apart from the radius values, there is a selection for the shapes of the integration area and the background (see the paper about the Spot Tracker [1]):



- *Concentric Circles* means that the integration area is a circular disk and the background intensity is averaged over a circular ring with outer radius √2 times the radius of the integration circle. This option is best if spots are very close at high energies, and it also provides the best suppression of local variations in the diffuse background intensity due to scattering by phonons.

- *Oval background* also uses a circular integration disk, but an elliptical outer border of the background area, with a semi-major axis twice the radius of the integration circle and the semi-minor axis equal to that radius. (The background area has the shape of two large ears.) This option is best in the case of a background intensity varying with the distance from the screen center and it also maximizes the energy range that can be evaluated for most spots, as the background area does



not touch the inner or outer border when the circular background would already touch it.
- *Azimuth blur* is for spots blurred in azimuthal (tangential) direction, due to small variations of the azimuthal orientation of the domains or crystallites. In this case, the integration disk is an ellipse with the semiminor axis being the radius defined above. The semimajor axis is oriented in tangential direction [perpendicular to the direction to the (0,0) spot] and gets enlarged to fit the azimuthal blur angle entered. For near-circular spots [near the (0,0) spot], the background area has a circular outer border, with $\sqrt{2}\cdot$`radius`. With increasing ellipticity (integration ellipse elongated in tangential direction) the outer background radius remains constant as long as the integration ellipse fits inside the circular background outline. Then the background outline becomes stretched in tangential direction, i.e., it becomes an ellipse. The total area remains $\sqrt{2}$ times the integration area, thus the background area is about 41% of the integration area. The background intensity is measured near the borders in the radial direction from the spot. Thus, the background intensity is sensitive to nonlinear background variations over the radius, but insensitive to neighboring spots in the azimuthal direction. (This is the opposite to the oval background, where the background is evaluated in tangential direction from the spot.)

For both *Oval background* and *Azimuth blur*, note that there is no thorough checking for whether the background area of a spot overlaps with the integration disk of any of its neighbors. Thus, use these modes only if the spots are well-separated up to the highest energy.

The size and type of the integration and background areas are indicated in the top right corner of the "SpotTracking" movie.

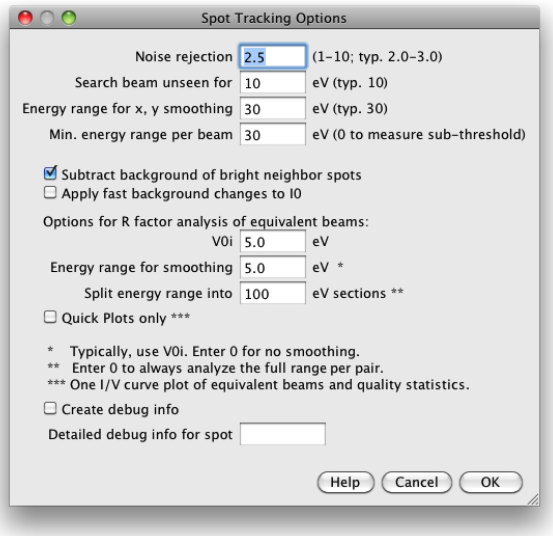
Track Spots

Starts spot tracking and intensity measurements (may take up to a minute). Tracking starts at the energy where the spot indices have been entered via *Set Indices*, then the program tries to follow the beams and to discover other beams listed in the pattern file if they become visible.

The numeric values of the parameters determining the tracking process can be usually left at their defaults. (When not measuring as a function of energy, the numeric parameters given in 'eV' below rather refer to the number of frames, i.e., data points of the output.)

Noise Rejection (default 2.5):

Determines how strong a spot must be to be taken as valid. The value sets the threshold of the significance (red curve in the position deviation plot generated by spot tracking). Increase this value if spots get trapped by screen inhomogeneities during tracking or if spot tracking finds spots where there are none at any energy. If the noise threshold is too low, stray spots might also wander into another (real, but weak) spot, inducing deletion of that spot.



Search beam unseen for (default 10 eV):

If a beam has not been detected over an energy interval of more than this value, information about its deviation from the predicted position is discarded and the program tries to find it as if it had not been detected before.

Energy range for x, y smoothing (default 30 eV):

Before measuring intensities, the deviations of the spot positions from the predicted value are smoothed, to obtain a continuous movement of the integration circle. A larger value of this parameter results in smoother movement of the integration circle. In case of local distortions of the LEED pattern, a large value may result in inaccurate positions, however. Measurements down to very low energies (<30 eV) may require a smaller value for this parameter. This parameter also determines how far the position may be extrapolated from the first/last detection of a spot. (Set 'Min. energy range per beam', below, to 0 for unlimited extrapolation.)

Min. energy range per beam (default 30 eV):

Beams with a total energy range less than this limit are ignored. When this parameter is set to 0 there is no such limit, and the program tries to measure all spots in the spot pattern file, irrespective of whether they are above the significance threshold. (see 'Noise Rejection', above.) Then, for spots that are below the noise threshold at all energies, the positions are inferred from the neighboring stronger spots. This is useful, e.g., for checking whether minority areas with a given superstructure are present. In this case, check the positions and make sure you don't mistake small background variations for a real signal.

Subtract background of bright neighbor spots:

Since spots often have a long-range background (tails of the spot profile), the background for nearby spots is not uniform. Use this option only if the spots show circular symmetry, not for elongated spots. This option fits a $1/r^2$ background in the vicinity of bright spots and subtracts that background before evaluating the intensity of weaker spots. This option is not available if spot shape 'Azimuth blur' is selected. Depending on the spot profiles, for good results, this option may need a larger integration radius than the lower limit of twice the measured spot radii. The background-subtracted stack will be displayed and can be examined if 'Create debug info' is selected.

Apply fast background changes to I0:

This option is only present if the measured beam current I_0 is available and I_0 smoothing is on, see *Set Energies, I0, t*. It measures the average background intensity and corrects the (processed) beam currents based on fast fluctuations of the background intensity. In this context, 'fast' means fluctuations that would be filtered out by smoothing of I_0. This option is useful if the background intensity can be determined with less noise than I_0. Typically, only fast variations of the background intensity are due to I_0 variations, slower changes of the background are due to energy-dependent scattering. This option works well if the background intensity is high (temperature > Debye temperature), I_0 smoothing is not much more than 5 eV/ΔE (where ΔE is the energy step), and if dark frames are available, i.e., when zero light corresponds to a pixel value of zero. The ViPErLEED hardware measures I_0 with very low noise; for such data it may be better to disable I_0 smoothing in case of I_0 jumps instead of using this option. To examine whether this option works well, plot the processed I_0 vs. (raw) I_0 with *More>>Plot...* after spot tracking and check whether the processed I_0 is less noisy than the raw I_0. You can also plot the background intensity divided by the (unsmoothed, but I_{00}-corrected) I_0. Use the *Apply*

fast background changes to I0 option only if background/I0 is substantially more noisy (with logarithmic *y* axis) than the background intensity.

The other parameters in this Spot Tracking Options dialog only affect the quality statistics plot for analysis of equivalent beams; these options are only available for $I(V)$ measurements, not for, e.g., time-dependent measurements. These are the V_{0i} parameter of Pendry's R factor (strictly speaking, its absolute value), the smoothing before calculating R factors (default 5 eV), and the energy ranges handled separately (default 100 eV): $I(V)$ curves are split into regions roughly this size, and for statistics, the R factor between symmetry-equivalent beams is evaluated for each of these regions. (Splitting into ~100 eV sections is done because the intensities of the low- and high-energy regions are often very different; the plot shows mutual R factors vs. intensity.)

One can also decide to create only two quick plots (Selected IV Curves and $I(V)$ Quality Statistics) instead of all plots. For large datasets, this avoids the time-consuming creation of large plot stacks. This is useful if the analysis is only meant to check the alignment of the sample, i.e., whether the $I(V)$ curves of equivalent beams agree, or the impact of different parameter values on the quality of the result. (When saving the data and 'Save Plots' is selected, the full set of plots will be saved irrespective of the *Quick plot only* setting.)

Spot tracking sometimes creates a window named `WARNING: Beam(s) uncertain (highlighted).` In this case, check these beams (marked by thick light blue circles in the main spot-tracker image stack; you may have to set an appropriate energy to see them) and use More>>Delete highlighted beams if appropriate. This warning may also come up if spot tracking has worked well, but the choice of the energy for Set Indices did not allow the program to determine a good model for the distortions of the LEED pattern.

Spot tracking creates several plots:

Selected I(V) Curves

If there are symmetry-equivalent beams, a plot of one set of such beams. This is mainly for judging the alignment and residual electric and magnetic fields. (The selection criteria for this set of curves are a large common energy range, a large number of equivalent beams, and high intensity.)

I(V) Curves

The stack of all $I(V)$ curves extracted. Note that the beam groups are in square brackets; $I(V)$ curves belonging to the same group should agree (symmetry-equivalent beams). Negative group numbers denote symmetry-forbidden beams; these may have a finite (true or apparent) intensity, e.g., due to deviations from perpendicular incidence or an uneven background.

Spot X/Y Deviations

For each beam, a plot with the deviations of the measured spot position from the position expected (as a function of energy), and this curve after smoothing as defined by the *Energy range for x, y smoothing* parameter. The smoothed deviations are used to obtain the positions of the integration disks for intensity measurement. Especially if the density of spots is high or there are defects on the screen, these plots should be examined to check whether spot tracking has been successful. A large jump or a position “running away” from a certain energy on will indicate a problem with tracking. These plots also include a line with the 'significance' of the spots, i.e., the value used to determine whether a spot is above the noise threshold (below the threshold, the significance is plotted as 0).

Spot Radii

A scatter plot with all spot sizes measured, as a function of energy. In case of a superstructure, the superstructure spots are marked by different colors than the integer ones. The spots are assumed to be ellipses; the extension in radial and tangential direction is plotted. Here, 'radial' refers to the direction to the screen center, except for “azimuth blur” mode, where the radial direction is defined as the direction to the (0,0) spot. The spot size plotted is an approximation to the standard deviation σ of a Gaussian peak. Since the peaks are usually not Gaussians, the sizes depend somewhat on the integration radius. The plot also shows a line with half the integration radius; it should trace the center of the point cloud or be at larger radius values than the center line of the cloud. Ignore the outliers, these are usually very weak spots. In “azimuth blur” mode, the tangential size of the spots is scaled down, as if the image was distorted to make the integration ellipses circular. Nevertheless, in “azimuth blur” mode, this criterion is mainly relevant for the size σ in the radial direction. It is less important in the azimuthal direction because the background area does not extend from the ellipse in azimuthal direction. See *Set Integration Radius*.

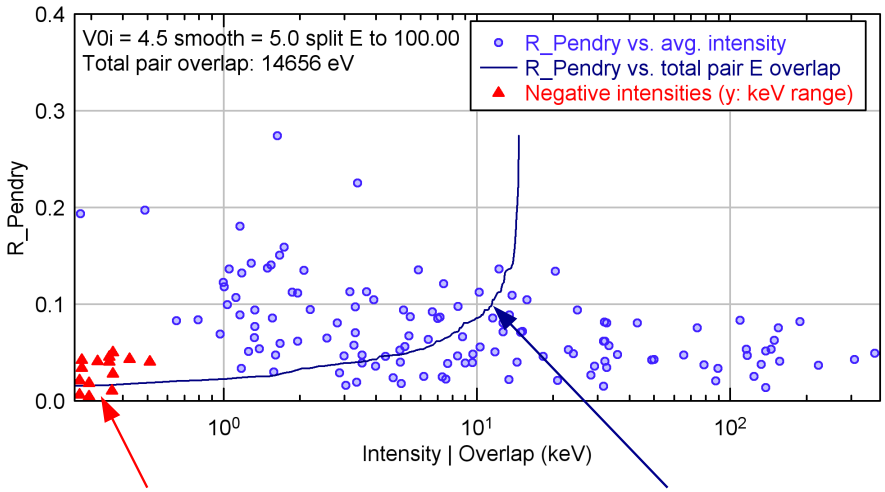
I(V) Quality Statistics

This plot shows the *R* factors between symmetry-equivalent beams in various ways:

(1) A scatter plot, where the horizontal axis is the average intensity of the *I*(*V*) curve or section of that curve (normalized to 1000 for the highest intensity occurring anywhere). Typically, due to noise, weak beams have higher R factors between symmetry-equivalent beams, i.e., the point cloud is "higher" on the left side of the plot. If the experiment was done very well (no residual magnetic fields, sample surface exactly normal to the electron beam), the points for the highest intensities will have mutual *R* values of less than 0.1.

(2) A line that shows the *R* factor against the cumulative energy range of all curve-section pairs with an *R* factor better than the given number. (If there are many symmetry-equivalent beams, this is more than the energy range available up to that *R* factor because many pairs can be selected from one group of beams.) Beams where no symmetry-equivalent curves are available are ignored.

(3) If there are beams with negative intensities (after smoothing), the plot shows red triangles: For these points, the *x* axis gives the absolute value of the most negative intensity, and the *y* axis gives the total energy range (per beam) where the intensity is negative. Thus, the red symbols, if any, should be as far to the bottom left as possible.



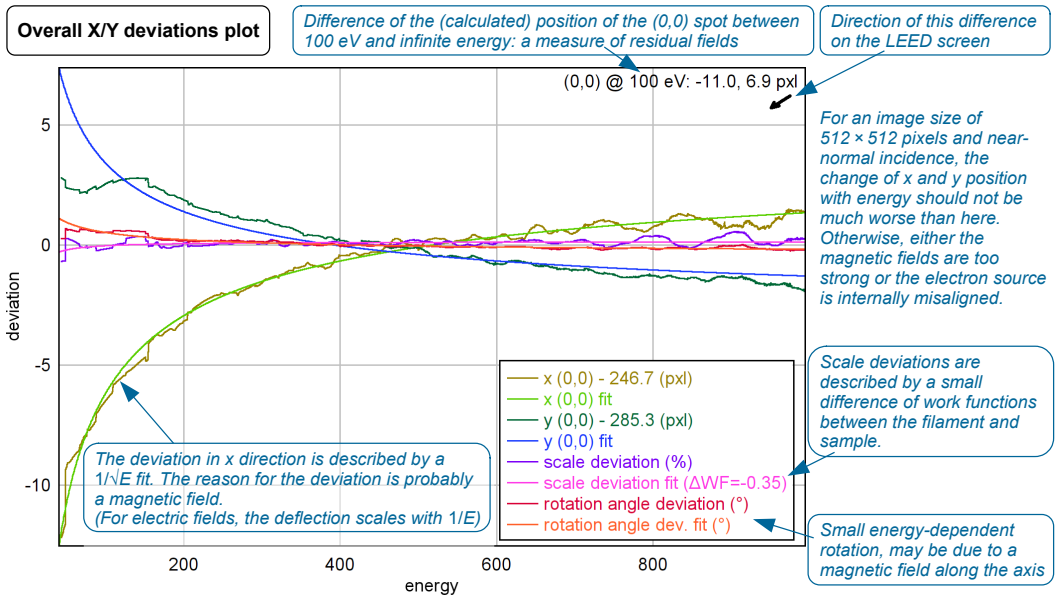
Markers for regions with negative intensity in *I*(*V*) curves. Should be only at the bottom left.

Symmetry-equivalent pairs with mutual R_P < 0.1 encompass a total energy range of 1.15×10^1 keV.

Overall X/Y Deviations

This plot contains information on systematic deviations of the spot positions from the expected position. It is based on 2D linear regression of the measured vs. expected position. This fitting procedure yields an estimated position of the (0,0) spot (which is usually hidden by the electron source). An energy dependence of the (0,0) position can be caused by, e.g., residual (magnetic) fields or an off-axis position of the filament in the electron source. The text and arrow at the top right indicate the displacement of the (0,0) spot at 100 eV vs. the extrapolated position at infinite energies (where the electron beam is not deflected). This calculation assumes magnetic fields, which yield a deflection proportional to $1/\sqrt{E}$. The direction of the arrow marks the direction of the movement of the (0,0) spot in the "SpotTracking" movie with decreasing energy. (This is valid unless the plot window is resized, which would distort the plot area and, hence, the arrow.)

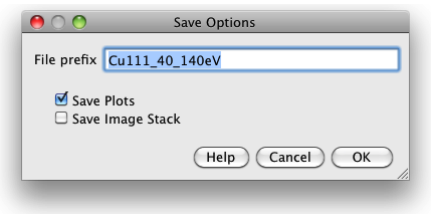
The plot also contains a line for the deviation of the scale factor (with respect to the usual $1/\sqrt{E}$ scale) from 100%. Small scale deviations can be due to the difference of the work functions of the filament and that of the sample and its surrounding. There is also a fit line for the scale factor, which assumes that deviations are due to such work function differences. For conventional LEED optics without additional electric fields, large scale deviations (more than ~2–3% at 50 eV) may indicate surface charging. The deviation of the scale factor is usually much larger for MCP-LEED, where fringe-field electrodes are present.



Save Data

Saves the results as csv files in a directory chosen by the user.

The user can choose a prefix (all file names start with this) and also select whether to save plots (as created by *Track Spots*) and the processed image stack (usually a big file).



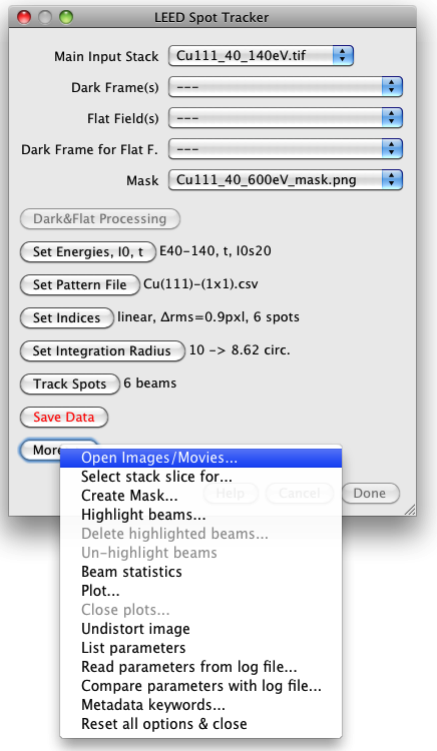
Files created:

- The main outcome: The intensities, corrected for the (processed) beam current I_0, file `<prefix>_IVcurves.csv`. This file should be processed with the LEED I(V) Curve Editor to create the experimental $I(V)$ curves used for comparison with the calculated ones.
- The uncorrected intensities (not taking I_0 into account) are written into `_rawInt.csv`. For all beams tracked, also the following information is written as `.csv` files: The x and y positions (in pixels) as well as the raw and smoothed deviations of the positions from the expected ones (`_x`, `_y`, `_dx_raw`, `_dy_raw`, `_dx_smooth`, `_dy_smooth`), the significance (set to ≈0 when it is below the noise threshold; file `_signif`), the spot radii in radial and tangential direction (`_rSize`, `_tSize`; see *Spot Radii*), as well as the intensity in the background region around the integration area and its standard deviation (`_backgr`, `_bsigma`).
- A `_log.txt` file, which contains the parameters used for spot tracking.
- If *Save Plots* is selected, one file for each of the plots mentioned in the *Track Spots* help is saved.
- If *Save Stack* is selected, the 'spotTracking' image stack is svaed, i.e., the input with dark/flat corrections applied and labeled integration circles (a large file). Otherwise, one image with beam-index designations (`spotIndicesImage.tif.zip`) is saved (at the energy of *Set Indices*). The image or stack is saved in `.tif.zip` format. It should be opened in ImageJ without prior unpacking.

More>> Popup Menu

Open Images/Movies...

Displays a dialog for opening the input files. Files selected as input that do not fit the requirements (e.g., wrong size, or a mask that is not a binary image) will be opened, but not selected as the respective input. Opening all files using this command is usually more convenient than opening and selecting them individually. If your computer does not have enough RAM for all image stacks (including the processed one, after dark-frame and flat-field correction), select "Virtual Stack". Then only the images currently required will be read from disk.



Select stack slice for...

Asks the user for the energy (or other x-axis variable, e.g., time; see *Set Energies, I0, t*) and selects the stack slice (i.e., the image) for this energy.

Create mask...

Facilitates creating a mask for a stack of LEED images. If a flat field is available, the tool is based on the flat field as an input (averaging over the stack slices); otherwise it uses the main input stack (the standard deviation of the intensity vs. energy for each pixel). There are two sliders: Initially, move the threshold slider to obtain a smooth outline of the screen area and of the edge of the electron source (with the arm holding it). In the second step, you may shrink or grow that area by a few pixels to refine it. In addition, if the program can guess the outline of the LEED screen, you can select "Limit to elliptical fit" and you can

try the checkbox to correct for the radius dependence of the intensity, which is typically present in the input images. To evaluate the result, you may use *Image>Adjust>Brightness&Contrast* to better see the border of the LEED image in the "SpotTracking" stack. When done, select the mask created in the main Spot Tracker panel. If required, use the standard ImageJ selection tools (oval, polygon, freehand) and the *Edit>Fill, Clear* and *Clear Outside* commands to further refine the mask.

Highlight beams...

Shows the selected beam(s) with a thicker circle. Useful in case of complex superstructures and to delete these from the output (see *Delete highlighted beams...*, below).

Delete highlighted beams...

Deletes these beams completely or in a given energy range. These beams will not appear in the output of a successive Save Data operation (but they remain circled and named in the stack). One cannot undo deletion except by running Track Spots again.

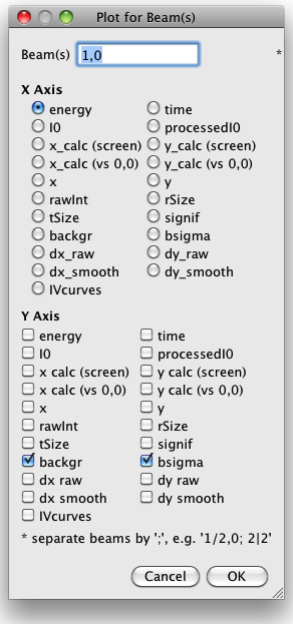
Un-highlight beams

Restores normal view after *Highlight beams*.

Beam statistics

Creates a table with one line for each beam successfully tracked: Beam group, number of data points, energy of the first and last data point, highest significance, and the energy where the highest significance is achieved. There is also a summary line with the total numbers and overall minima/maxima.

Plot...



Creates a plot of various data available. Examples include (processed) I0 or data for the beam(s) requested, such as intensity. See the list of .csv files in *Save Data* for the items available.

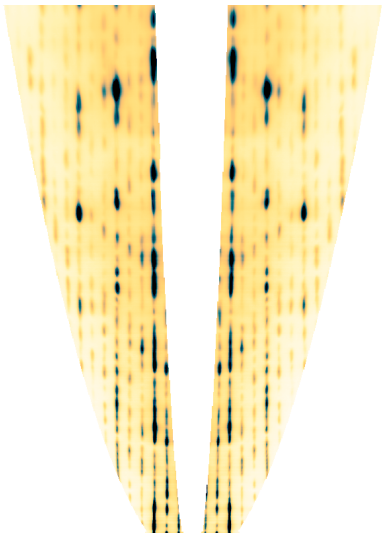
Close plots...

Closes all or a given subset of plots created by *Track Spots*.

Undistort image/stack

Uses the "Spot Tracking" stack as an input and applies the distortion corrections determined when the spot indices were set. The undistorted image has the position of the (0,0) spot at the center. If the outer border of the LEED screen in the undistorted image is far from elliptical this indicates that there have not been enough spots close to the border to correctly determine the distortions. The user can select whether to apply the correction only to the current slice (the image currently shown) or the whole stack. In the latter case, except for LEEM mode, there are two options for the image scale: "scale like input" creates a stack where the spots are moving as in the input, while "fixed k-space scale" de-magnifies low-energy images such that the spots of a given beam are always at the same pixel position. Stack undistortion should be run after spot tracking; then the overall deviations caused by residual fields are taken into account. The output can be normalized, by dividing by the processed I_0 (if available), to eliminate brightness variations due to changes of the incident electron beam current. The output of stack undistortion is a virtual stack with caching. Thus, the images are created only when needed. This means that the output is quickly visible, but some image operations using the

undistorted output will be initially slow, until all slices of that stack have been created. This also means that the stack created may become partly or fully unavailable when one of the input images/stacks is closed. Note that averaging over the slices of an undistorted stack (*Image>Stacks>Z Project…*) requires ImageJ version 1.54j or later. Further processing of the undistorted stack (e.g., background subtraction, resizing) requires that you duplicate this stack.



Averaging over a range of energies of the undistorted stack with fixed k-space scale is handy to search for weak spots that may be hard to detect in individual slices due to modulations by the grid and noise. One can also create sections through k space with the energy axis up, using *Image>Stacks>Reslice [/]…* (see the figure for an example).

List parameters

Creates a table with all numeric parameters; mainly for debugging. When in macro-recording mode (*Plugins>Macros>Record…*), also writes the macro commands for setting all parameter values to the Recorder window.

Read parameters from log file...

Reads all parameters from a user-selectable file, usually a `_log.txt` file saved in a previous spot-tracking session. (Experts might also modify the machine-readable part of such a log file to create a setup file; better use a macro for this.)

Compare parameters with log file...

Reads all numeric parameters from a user-selectable file, usually a `_log.txt` file saved in a previous spot-tracking session, and compares it with the parameters of the current session (shows a table of differences).

Metadata keywords...

Defines the names (case-sensitive) of data columns for energy, I_0, ... in the input files. Separate multiple possibilities with a vertical bar. The keywords should be the full prefix, as it appears below the window title in the 'SpotTracking' stack, including the '=' sign. Example: '`energy=|E=|V=`' allows 'E=123.5' but not 'Energy=123.5'.

Reset all options & close

Resets all options and parameters to their default settings and closes the Spot Tracker.

Good to Know

On the main ViPErLEED Spot Tracker panel, red color usually indicates where user interaction is required next.

The `Enter` key brings the main ImageJ panel to the foreground. When the Spot Tracker panel is in the foreground, `SHIFT-Enter` brings the “SpotTracking” image stack to the foreground.

In ImageJ, *slices* are the single images that an *image stack* (e.g., a movie) consists of. Keyboard shortcuts for moving to the previous/next slice are ',' or '<', and '.' or '>', respectively. You can also use the mouse wheel.

Right-click on the animation (play) symbol at the bottom left to change the speed of playing a movie (it may be slower than the speed in frames per second, fps, if calculating the frames takes time).

If you have a movie with strong brightness variations, you may try setting 'Auto contrast stacks' in *Edit>Options>Appearance…* Bright spots will appear saturated, but you may better see the faint ones.

Why is there a `(V)` at the end of title of many image stacks? The `(V)` stands for *virtual stack*, i.e., the images are not in memory but read from disk or calculated on the fly if required. The stack named `..._SpotTracking` (created by the ViPErLEED Spot Tracker) is a virtual stack with caching; its slices are kept in memory as long as there is sufficient memory. You can click on the status line at the bottom of the main ImageJ toolbar to see the used and total memory. Use *Edit>Options>Memory&Threads…* to change the maximum amount of memory allocated to ImageJ (requires restarting ImageJ thereafter; make sure you allocate less than the RAM available in your computer).

If you get an error message saying that all memory has been used, it may help to add

```
-XX:SoftRefLRUPolicyMSPerMB=100
```

to the options for the Java Virtual Machine (JVM). These options are in the `ImageJ.cfg` file in the ImageJ folder. On MacOS, these options are in the `info.plist` inside the ImageJ package: Right-click on ImageJ in the Finder and select *Show package contents*. The same command with a value of 10 instead of 100 would be even stronger, telling Java to be very restrictive with memory spent for caches. The downside is that this will usually lead to longer execution times.

ImageJ can save images (also image stacks and plots) as `.zip` files. These are compressed `.tif` files that can be directly opened in ImageJ without unpacking (also by drag&drop onto the status line of the main ImageJ panel). *I*(*V*) movies recorded as ViPErLEED `.zip` archives can NOT be opened by the ImageJ *File>Open* command (or drag&drop on the status line); use *Open LEED Movie* or *More>>Open images/movies* for these.
The file types `.tif` and `.zip` are the preferred formats for saving, since they contain the full information and image resolution. The mask can be also saved as `.png` file. **NEVER** save images as `.jpg` unless they are meant for illustration only; even then mind that `.jpg` has usually very poor quality for sharp borders, especially for lines, text, etc.

Single plots (but not stacks of plots) can be modified, e.g., one can zoom into a rectangle selection with the '+' key, and reset the range with the gray 'R' appearing under the mouse pointer in the bottom left-corner. With the mouse over the left or lower border, there are also other gray symbols; their meaning is explained in the help text appearing in the status line of the plot when the mouse cursor is above such a symbol.
You can set the default size of plots (and final size of plot stacks) with *Edit>Options>Plots…*

Many functions of the LEED Spot Tracker can be controlled and automated via the ImageJ macro language. Record macro commands with *Plugins>Macros>Record…*

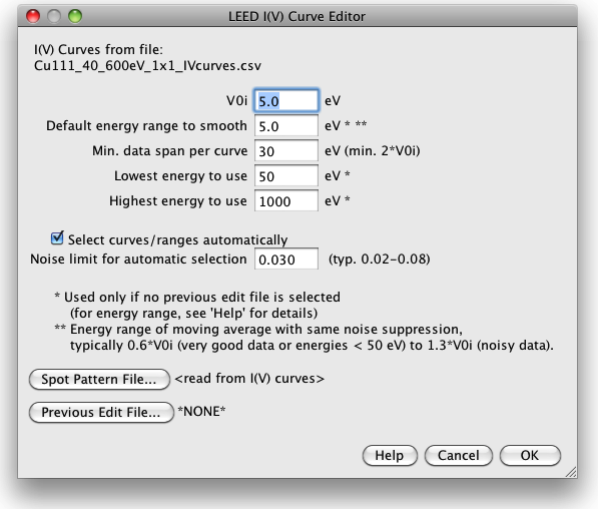
For smoothing in ViPErLEED, the strength of smoothing is given as the inverse square of the noise gain for white noise. E.g., '9 points' means that smoothing will reduce white noise to approximately 1/3 of its original value. This corresponds to the noise suppression of a moving average over 9 points. The actual smoothing algorithm averages over more points with a weight function. For I_0 data and *I*(*V*) curves a modified sinc smoother [2] is used.

ViPErLEED I(V) Curve Editor

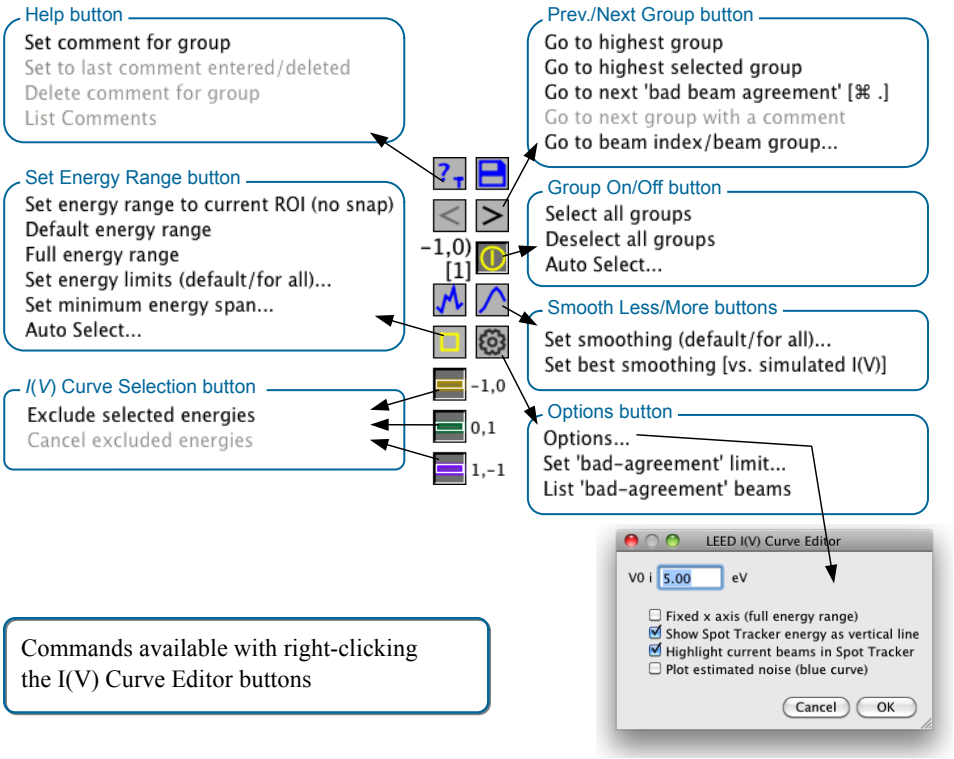
Parameters and Settings for the ViPErLEED I(V) Curve Editor

Initially, the I(V) Curve Editor asks for an input file with the $I(V)$ curves. The following menu determines the settings.

- **V0i**: Imaginary part of the inner potential (strictly speaking, its absolute value), needed for calculating the R factor. When averaging symmetry-equivalent curves that do not all include the full energy range, V_{0i} also determines the width of the transition zone with smooth fade in/fade out. If V_{0i} is not known, use, e.g., a value of 5 eV.



- **Default energy range to smooth**: How much the curves should be smoothed; this is the energy range of a moving average with same noise suppression, typically 0.6 V_{0i} (very good data or data including low energies < 50 eV) to 1.3 V_{0i} (noisy data). If a previous edit file is used, this setting has no effect and the value from the previous session is used.
- **Min. data range per curve**: Curves with fewer contiguous data points than this are ignored. Note that you cannot make ignored curves (with too few points) visible any more in the current editing session. You have to close and open the Curve Editor to get them back.
- **Lowest energy to use** and **Highest energy to use**: The default energy range if a beam is selected for the first time. These parameters also limit the range for automatic (noise-dependent) selection of energy ranges. The limits do not restrict manual selection in the I(V) curve editor. If a previous edit file is used, the settings for the default energy range from the previous session are used, also for curves not selected in that session.
- **Select curves/ranges automatically**: Automatically selects which groups of symmetry-equivalent $I(V)$ curves and which energy ranges will be selected. This selection is mainly based on an estimation of the noise and its impact on the R factor.
- **Noise limit**: Automatic selection is done such that the estimated impact on the R factor is less than the noise limit given. Typical values are around 0.05; lower values are more selective, higher values lead to a larger total energy range (larger 'database'), at the cost of increased noise.
- **Pattern file**: Usually, the information on symmetry-equivalent beams is read from the headings of the file with the $I(V)$ curves (spot groups in square brackets). If this is not the case or you want to use a different symmetry, a spot pattern file can be specified. A spot pattern file is a comma-separated list (.csv file) of beam names, h, k, g_x, g_y (reciprocal lattice vector in Cartesian coordinates), and beam group number (equal for symmetry-equivalent beams). Such a file can be created with the pattern simulator of the ViPErLEED GUI.



- **Previous edit file**: If these *I*(*V*) data have been edited previously, one may select the file from the previous session to continue with the same selection of curves, energy ranges and smoothing. If an edit file is selected and you want a fresh start (not continue the session stored in a that edit file), press the button to open the file dialog and then <Cancel>.

  If *Select curves/ranges automatically* is checked, automatic selection will supersede the selection in the edit file; only the smoothing (and deselection of individual curves from the average) will be read from the edit file.

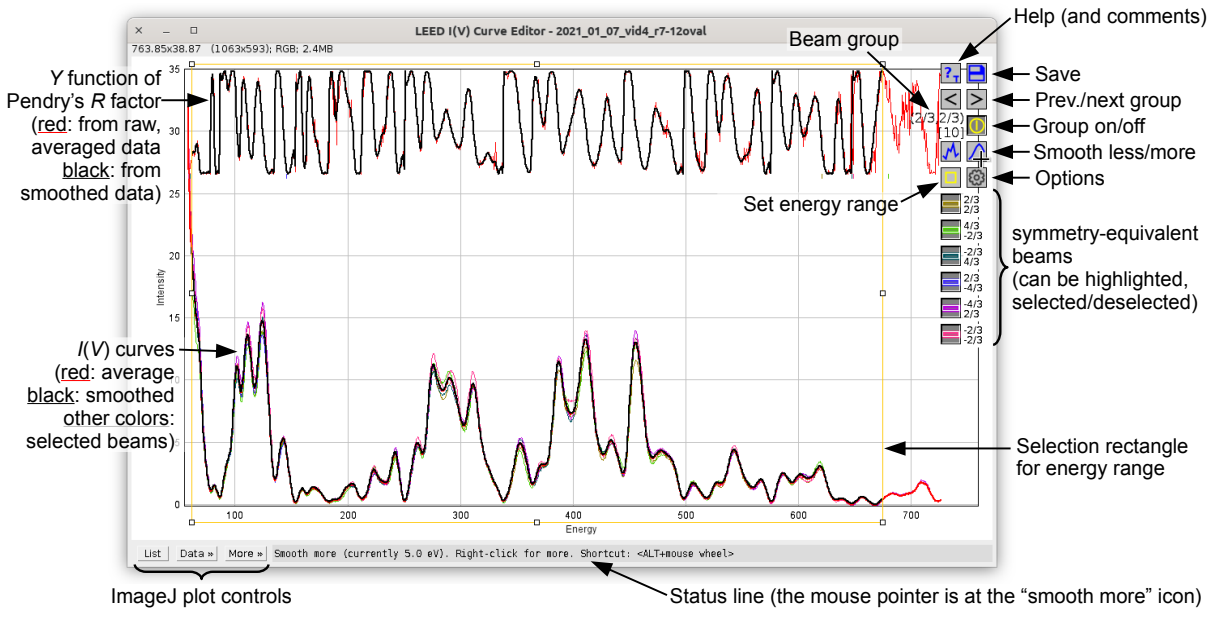
Main Plot

- The **main part** of the plot area shows the $I(V)$ curve(s) of a group of symmetry-equivalent beams, their average (red) and the smoothed average in the selected range (black).
- The **top part** of the plot area shows the Y function (modified logarithmic derivative used in Pendry's R factor), for the averaged $I(V)$ curve (red) and the smoothed $I(V)$ curve (black). This is the function that is compared to the corresponding function of the calculated $I(V)$ curves.
- Small, colored **ticks** below the Y function indicate the limits of the data ranges of the individual $I(V)$ curves. Thicker and longer ticks indicate an excluded energy range of an input beam.

Buttons

- **Help** ('?' symbol) Shows the help window (this text). Right-click to set or modify a **comment** (annotation) for the current group of symmetry-equivalent beams. (This is indicated by the small 'T' symbol.) Comments are saved in the edit file.
- **Save** saves the `.csv` file with the final curves. Right-click to save the data without smoothing.
- The **<** and **>** buttons switch to the previous/next group of symmetry-equivalent beams. Keyboard shortcut: '<' or ',' and '>' or '.' (on non-English keyboards, ',' and '.' keys work only if this is the main function of the key, without pressing the shift key). The <Page Up>, <Page Down>, <Home>, and <End> keys also work. Alternatively, you can use the mouse wheel.

  Right-click the '<' or '>' symbols for more navigation options: First, last, or last selected beam group. You can also jump to the previous or next beam group with a comment, or previous or next group with bad agreement of equivalent beams (for the latter, only selected groups and energy ranges count). You can also enter the beam indices or group number for jumping to a group.
- **Group On/Off** selects whether the curves of the currently shown group of symmetry-equivalent beams should be used at all. When selecting a group, the energy range is set to the last range selected (or to the limits, if it was never selected before).
  Keyboard shortcut: SPACE bar.



Right-click to select or deselect all groups. (Note that *Select all groups* does not select groups where the energy span is less than the minimum span.)

The *Auto Select* function available via right-clicking does not only switch groups on/off but also selects energy ranges, maximizing a figure of merit that depends on the noise.

- **Smooth More/Less** selects how strongly the curve (or average of curves) will be smoothed. You can modify smoothing also with the <ALT> key down and the mouse wheel. Press <SHIFT> for a faster change.

  Right-click to change the (default) smoothing for all deselected (switched-off) groups or to apply a given smoothing value to all selected groups (or the current group and all higher groups). When applying the smoothing value, you can select *noise-dependent smoothing*. This option sets slightly stronger smoothing for curves that are more noisy than the currently selected one, and slightly weaker smoothing for less noisy curves.

  The *Set best smoothing [vs. simulated I(V)]* option asks for a file of simulated *I*(*V*) curves (`THEOBEAMS.csv` file). It then tries different smoothing parameters to find the smoothing that results in the lowest *R* factor between smoothed experimental and simulated curves, and applies this smoothing. This should be done only as the very last step, after refinement of the structure and inner potential.
- **Set Energy Range** (yellow rectangle): Use the ImageJ Rectangle tool from the main ImageJ Toolbar to select the energy range and then press this button.
  Keyboard shortcut: '#' or '0'

  Only the left and right sides of the selection rectangle are taken into account. When the left or right side is close to the limit of one of the input curves, and a slight shift of the boundary would avoid the necessity to smoothly fade in or fade out that curve, the range snaps to this point. You can override the snap with a right-click on the *Set Energy Range* button and *Set energy range to current ROI (no snap)*.

  For a given beam group, only one energy range can be selected. In other words, you can't have a gap in the output data. (This restriction is required by TensErLEED, which is used as a backend for LEED-*I*(*V*) calculations in `viperleed.calc`.)

  When there is no selection and the *Set Energy Range* (yellow rectangle) button is pressed, the default energy range is used. This is defined by the limits from the dialog window shown when opening the Curve Editor, unless it has been modified by *Set energy limits* from the context menu of the *Set Energy Range* button. Pressing the *Set Energy Range* button also selects a curve if it was deselected.

  By right-clicking the *Set Energy Range* button, one can also set the full energy range for the curve or the default energy range (as given by the limits). You can also modify these limits (the default energy range) or the minimum energy span (previously specified in the starting dialog), and optionally restrict the energy ranges of all groups to obey the new limits. **Automatic selection** of beam groups and energy ranges (depending on the noise) is also available from this context menu.

  Hints for manual selection - Select regions where the *Y* function at the top of the plot is not too noisy. If there is no sufficiently long low-noise range, deselect the whole curve. Rule of thumb: For 0.5 eV energy steps, in the ideal case, the noise (peak–peak) should be on average less than ~20–30% of the full vertical range of the Y function. Select the high-energy limit such that high-energy

regions with an average noise larger than this noise are excluded.

If symmetry-equivalent beams differ substantially in the low-energy region, exclude these low energies. Deviations between symmetry-equivalent beams at low energies only are typically due to residual magnetic fields; deviations at all energies are more likely due deviations from normal incidence. Very large deviations may indicate that you have the wrong spot pattern file, i.e., the symmetry is wrong.

- **Options** (gearwheel symbol): Use the *Options...* dialog to change the V_{0i} value (used for calculating the Y curves at the top of the plot and for any R factors), to use a fixed x axis with the full energy range for all curves, or to show also a noise estimate on the plot (blue). When the noise is plotted, the y scale for this curve is always fixed (range 0–0.25) and the blue horizontal line is the noise limit for automatic selection.

  The *Options...* dialog also lets you **synchronize** the current I(V) Curve Editor with the **'SpotTracking'** display of the Spot Tracker: This shows the current energy of the Spot Tracker as a black vertical line in the I(V) Curve Editor. The beams of the current beam group in the I(V) Curve Editor can be highlighted in the Spot Tracker (unless the highlighted beams of the Spot Tracker still mark the dubious beams of spot tracking; these are not modified).

  By right-clicking the 'Options' button, you can select the threshold for classifying '**bad agreement**' of symmetry-equivalent beams and create a list of these 'bad-agreement' beams. A typical value for this threshold is between the threshold value for automatic selection and twice that value. 'Bad agreement' is based on a 'local R factor' (within a small energy window) between the beam and the average of all selected beams. Note that Pendry's R factor is very sensitive at the minima, much less sensitive at the maxima. You can see the reason for the disagreement when moving the mouse over the button of the beam with 'bad agreement' and comparing its Y function to that of the average.

  You can also jump to the previous or next group with bad agreement by right-clicking the '≤' or '≥' button, respectively; energies of bad agreement are then flagged by thick, vertical lines.
  'Bad agreement' is analyzed only for selected beams and energy ranges.
- **Individual curve buttons** (colored '–' symbols): Press a button to select/deselect the curve of the respective beam (if more than one). You can highlight a curve by moving the mouse over the button. Then, the status line at the bottom shows the R factor of this beam vs. the average of the currently selected beams.

  If a beam has bad data in a given energy range (e.g., due to a dust grain on the LEED screen), select that range with the ImageJ rectangle tool (only the left and right side of the rectangle are taken into account). Then right-click the button for this beam and exclude this energy range with 'Exclude selected energies'. In the plot, the excluded energy range for a single beam is indicated by thick, long vertical lines below the Y function; then there is a 'Cancel excluded energies' command available with right-clicking the button for the respective curve.

Typical workflow

If you have taken more than one $I(V)$ movie for averaging, average their $I(V)$ curves before using the I(V) Curve Editor.

When opening the (averaged) $I(V)$ curve for the first time, start with **automatic selection** (also available later with right-clicking the on/off or *Set Energy Range* button) to select the energy ranges for all curves.

Automatic selection is based on an estimate of the noise of the curve and its impact on the *R* factor. Selection is done such that the average noise is less than the given noise limit and a figure of merit is optimized. The figure of merit increases with selected range and decreases with noise. Typical values for the noise limit are around 0.05; lower values are more selective, higher values lead to a larger total energy range (larger 'database'), at the cost of increased noise.

The next step is setting the **smoothing** value. Select a curve that starts at a medium energy and has medium noise. Then adjust the smoothing (e.g., using the mouse wheel with the <ALT> key pressed) such that 'real' features of the *I*(*V*) curves are preserved as best as possible while suppressing the noise. (Noise is often visible as wiggles in the smoothed *Y* curve where the *I*(*V*) curves have no apparent wiggles. These wiggles in the *Y* curve should be strongly attenuated.)

Then right-click on a smoothing button and apply the current smoothing to all curves, with 'noise-dependent smoothing' enabled. Check that the smoothing is not too strong for the first beam groups where low energies are included; if so, adjust smoothing for these groups. (Very sharp peaks at low energies mainly occur for 5d metals or if very low energies, below 50 eV, are included.)

Finally, check for **bad agreement** of symmetry-equivalent beams (CTRL-previous group, CTRL-next group[1]). The energy of the worst agreement of a given beam with the average will be marked by a vertical line. You may move the mouse over the button for this beam to compare its *Y* function with that of the average. Sometimes, the bad agreement is caused by a defect of the LEED screen (if only one out of many beams is an outlier) and a short section of the 'bad' beam can be excluded: Select the 'bad' energy range and exclude it for the beam by right-clicking on its button. In other cases, especially if such a 'bad' region is close to the ends of the energy range, it makes sense to set the energy range for the beam group such that the region of poor agreement is avoided. If many groups show large disagreement of the symmetry-equivalent beams, consider repeating the measurement with better adjustment of perpendicular incidence and/or better compensation of residual magnetic fields.

Finally, save the data. You can now use them as input for structure optimization (file `EXPBEAMS.csv`).

Towards the end of a LEED *I*(*V*) study, when you have a good best-fit model from the simulation calculations, you may want to try the 'Set best smoothing [vs. simulated *I*(*V*)]' option (right-click one of the smoothing buttons) for the last tweak (typically with 'noise-dependent smoothing' enabled). Usually, the improvement of the *R* factor will be marginal.

Good to know

Even if you do not save the final result, the Curve Editor keeps track of what you did and saves an 'Edit File' in the same directory as the input. If you close the window and open the editor again, it will propose to use that Edit File to continue.

When the mouse is above a button, the status line at the bottom (and the status line of the ImageJ toolbar) displays more information.

When the selected curves are averaged, they are first normalized and the slow trends of the intensity between the beginning and end of the overlap region are equalized. Additionally, if a curve starts or ends inside the selected energy range, smooth fade-in or fade-out is used to avoid jumps.

For zooming into the plot, select a rectangle and press the '+' key.
If the mouse pointer is to the left of the plot area or below it, gray symbols allow you to modify the plot limits (axis ranges). The 'R' at the bottom left resets the plot to the original limits, and arrow-like triangles near the ends of the axes allow you to shrink or extend the range. The 'F' ('full range, fit all') gets everything into the plot window, including energies where no data are available for the current curve(s). You can set a fixed energy range corresponding to this full range in the options.

If you want a different color for the selection rectangle, you can set it in ImageJ: *Edit>Options>Colors...*

You can have more than one I(V) Curve Editor window at the same time, to compare different sets of *I*(*V*) curves. These windows are synchronized, i.e., they show the same beam group (if available) and the same energy range on the *x* axis.

Smoothing is performed using a 4th-degree modified sinc smoother [2]. The best smoothing parameter is typically 0.6 V0i (very good data or energies < 50 eV) to 1.3 V0i (noisy data). The smoothing parameter value (in electronvolts) corresponds to the 'window length' of a moving-average filter with the same noise suppression for white noise. (The smoothing algorithm used preserves the shape of the *I*(*V*) curves much better than a moving-average filter with the same noise suppression.)

ViPErLEED Utilities

The **ViPErLEED Commands** window provides a quick way to access the commands. These commands are also available via the ImageJ menu *Plugins>ViPErLEED* or the ImageJ command finder (*Plugins>Utilities>Find Commands*, or type CTRL-L[1])

- **Open LEED Movie** opens a ViPErLEED movie stored as a .zip file or an 'AIDA' LEED movie (Automatic Image and Data Acquisition, EE2000/EE2010; `*.vid` format). LEED movies are shown as *Image Stacks* in ImageJ.
- **Average I(V) Curves** averages the *I*(*V*) data of up to six input files.
  If you have measured several LEED movies (at different distances to the sample), use this tool for averaging the *I*(*V*) curves, to reduce the noise (including the noise introduced by the grids). Thereafter, use the I(V) Curve Editor.
- **Stitch I(V) Curves** joins sets of *I*(*V*) curves that have different energy ranges (with a small overlap) and possibly different scale factors (e.g., camera gain, exposure time, etc.).
- **I(V) Curve Interpolation** interpolates data to different (usually finer[3]) energy steps. Also works if the energy axis has non-equidistant points (may be even descending since plugin version 1.02, but must be monotonous).
- **R Factor Between Data Sets** compares two files with *I*(*V*) curves and lists the *R* factor between them for each beam and the overall *R* factor. (Values obtained with `viperleed.calc` may be slightly different, due to subtle differences of the algorithms.)
- **I(V) Curve Quality Statistics** provides statistics for assessing the quality of *I*(*V*) measurements, such as *R* factors between symmetry-equivalent beams and negative intensities. This tool can create a list or a plot; the latter is the same as obtained from the Spot Tracker.

- **I(V) Curve Tools** can modify the intensities in *I*(*V*) curve files, extract a subset of the beams or an energy range, transform beam indices, and/or modify the information on symmetry-equivalent beams in *I*(*V*) curve files:
    - **Correct intensity values**: Modifies the intensity values. The function for modifiying the intensities should be specified in the ImageJ macro language. Variables 'I' (current intensity value) and 'E' (energy) are provided, and the result should be assigned to the variable 'I'. For simple expressions that do not contain '=' signs, 'if' clauses, etc., assignment to 'I' can be omitted, e.g. '`I/sqrt(E)`' is equivalent to '`I=I/sqrt(E)`' and divides all intensities by the square root of the energy.
      An energy-dependent correction can be used, e.g., to account for energy-dependent detection efficiency of a micro-channel plate in an MCP-LEED system. A typical correction like this might be '`Econv=80; I = I/(1-exp(-(E+Econv)/230));`' where '`Econv=80`' is the conversion voltage (the bias at the entrance side of the MCP). Of course, you can also put the value of Econv directly into the equation, e.g. '`I/(1-exp(-(E+80)/230));`'.
    - **Limit energy range**: Extracts the given energy range. Specify the energy range as, e.g., "`80-200`". Both limits are included.
    - **Extract beams**: Extracts only certain beams and omits the others. One can extract only integer beams, only superstructure beams, or the beams present (or not present) in a given file [some other .csv file with *I*(*V*) curves].
    - **Modify basis**: Applies a transformation matrix to the spot indices. You can select the new indices of the (1,0) and (0,1) spots. You can use this function, e.g., to swap the *h* and *k* indices: Change (1,0) to (0,1) and (0,1) to (1,0). Swapping *h* and *k* is often needed for crystals with threefold symmetry, where (1,0) and (0,1) are not equivalent, but it is initially not known which is which. If the spot labels have included group numbers in square brackets (to indicate the symmetry-equivalent beams, see below), these group numbers will be deleted.
    - **Modify groups of equivalent beams**: An *I*(*V*) curve file typically contains the *group number* for each beam. The group number is the number in square brackets in the name of the beam given in the heading. Beams with the same group number are considered symmetry-equivalent.
      These group numbers can be set to the values of a given spot pattern file, changed to a running index such that all beams are considered symmetry-inequivalent, or, alternatively, the group numbers can be deleted. (In the latter case, any future operations that require knowledge on symmetry-equivalent beams will ask for a spot pattern file.)

  You can select one or more of the functions in the above list.

Good to know

If you want to have the *ViPErLEED Commands* panel present when ImageJ starts, add

```
run("LEED Commands");
```

(with the semicolon) to the "AutoRun" macro of your `StartupMacros.txt` (or `StartupMacros.ijm`) file (in the ImageJ/macros directory) or to the list of startup commands by selecting *Edit>Options>Startup* from the ImageJ menu.

References

[1] M. Schmid, F. Kraushofer, A. M. Imre, T. Kißlinger, L. Hammer, U. Diebold, and M. Riva, *ViPErLEED package II: Spot tracking, extraction and processing of I(V) curves*, arXiv:2406.18413, Phys. Rev. Research (2024).

[2] M. Schmid, D. Rath, and U. Diebold, *Why and how Savitzky-Golay Filters should be replaced*, ACS Meas. Sci. Au **2**, 185 (2022).

FAQ

Spot Tracker Input Files

My LEED I(V) movie is a directory of single images, how should I name them?

In principle, it is enough if the energies are equidistant and the file names are sorted in the sequence of ascending energy.
You can then use *File>Import>Image Sequence*.
In the spot tracker, you can use *Set Energies, I0, t* to manually set the energy range.

If you want it a bit more comfortable, you can extract the energy from the file name. E.g. if your files are named like

```
20250211_Cu111_E150.5_I01.234_t67.8.tif
```

and all energy values are following the "`_E`" and all sample current values follow the "`_I`", you can use the spot tracker's *More>>Metadata keywords*. Have an energy key "`_E`". Same thing for beam current "`_I`", etc.

In the case of

```
myCrystal_150.tif
```

for 150 eV, a simple underscore "_" would be sufficent as energy key. Also `my_crystal_150.tif` is ok (with version 1.02 of the plugins), but not `Cu_111_150.tif`, since this would interpret "`111`" as the energy.

The default list of keys in the spot tracker for the energy is "`energy=|E=|V=`", which means that "`anytextE=150.5moretext`" or "`blahenergy=150.5blah`" etc. will work for decoding the energies.

Keys are case-sensitive.
Scientific format like "`E=1.505e+2`" or "`E=1.505e02`" is **not** supported; it would be read as "`E=1.505`".

I have color images, what should I do?

For an unclear reason, some OCI LEED systems were sold with a color camera. Since LEED screens emit only green light, 50% of the camera's pixels (the red and blue ones) remain essentially dark, so the camera sensitivity is reduced to half of what it would be with a monochrome camera.

If you have color images, usually you would use the green channel. (For a 3×8 bit RGB image, use *Image>Type>RGB stack* to see whether there is any useful information in R or B.)
The following ImageJ macro extracts the green channel from an 8-bit image or stack of 8-bit images:

```
setRGBWeights(0, 1, 0);  //green channel has 100% weight
run("8-bit");
```

Note that using 3×8 bit RGB images is not desirable, one should have a better pixel value resolution for good results, 12 or 16 bits.

Can I use images obtained with a consumer camera (DSLR camera, …)?

NEVER use jpeg images! Apart from the compression losses and the poor 8-bit pixel value resolution, they usually have a nonlinear intensity scale (gamma correction or an even more complicated function for sRGB).

Note that also other formats such as TIFF from consumer cameras may have a nonlinear relation between image intensity and pixel value.

To check whether your camera is linear, take images of the same object with two exposure times that differ by a factor of 4. The intensity difference between a bright (but not saturated) and a dark object should also scale by the same factor of 4.

Energy Calibration

What accuracy do I need?

For comparison with calculated LEED $I(V)$ curves and structure determination, the accuracy of the energy scale should be better than 0.5%, preferably around 0.1%. With most LEED controllers, the factor between the 0–10 V input for beam energy control and the actual beam energy is NOT sufficiently accurate. Also many handheld digital multimeters are not sufficiently accurate (check the specifications). The ViPErLEED hardware contains a high-voltage input for accurately measuring the filament voltage, used to calibrate the energy scale. If your LEED controller has no output for the filament high voltage, see the documentation of the ViPErLEED data acquisition system for how to access the filament voltage.

Do not care about a small offset between nominal and actual beam energy (up to a few eV); LEED $I(V)$ calculations will shift the energy axis if necessary.

My LEED controller has a nonlinear relationship between nominal and actual electron energy. What should I do?

The spot tracker also works if the energies are not evenly spaced (they must be ascending, however).

If you can determine the real filament voltage (e.g. by measuring the filament high voltage during the acquisition of the LEED movie[4]), it can be used as an input for the spot tracker. You can open a table (`.csv` or `.tsv` file[2]) with the actual beam energies in ImageJ and then select it with *Set Energies, I0, t*. The table must have one line for each image of the movie. If the true energies are available from the metadata of the LEED movie (shown in the status line at the top of the image stack, e.g. "`Emeas=150.5`") you can use the spot tracker's *More>>Metadata keywords* to define this as an energy key (in the case above, the key should be "`Emeas=`"). Then you can select "input stack" as a source from where to read the energies in *"Set Energies, I0, t"*.

The $I(V)$ curve editor needs equidistant energies. Interpolate the $I(V)$ curves obtained from the spot tracker to equidistant energies using the $I(V)$ curve interpolation utility. For interpolation, select an energy step that is not larger than the smallest step in the input file.[3]

Beam Current I_0

Do I need a measurement of I_0, and if so, why and how?

The current I_0 of the electron beam incident on the sample is used to normalize the intensities. For most LEED controllers (not for OCI controllers if configured to keep I_0 constant), I_0 depends on the electron energy. In addition, especially during warm-up, sudden jumps of the beam current occur due to stick-slip

motion inside the electron source. Note that the emission current displayed by many LEED controllers is not the same as I_0; the emission current is the total current emitted by the filament and also includes electrons that impinge on electrodes inside the electron source (e.g., the anode). Thus, the emission current is usually substantially higher than the beam current I_0.

If there are slow and smooth variations of I_0 over energy or time, it is not absolutely necessary to correct for changes of I_0 when the $I(V)$ curves are used for LEED $I(V)$ calculations. Pendry's R factor is insensitive to slow and smooth variations of a scale factor of the intensity. If the experimental intensities are not corrected for changes of I_0, substantial variations of I_0 may lead to a visually poor agreement between the measured and calculated $I(V)$ curves, however.

If the LEED controller does not keep I_0 constant and provides no means to measure I_0, during the $I(V)$ data acquisition, the ViPErLEED data acquisition system can measure the sample current with the sample biased to +33 V. The bias voltage is needed to suppress emission of secondary electrons, which would lead to an incorrect current determination. (Without sample bias the sample current can be negative or positive, depending on the secondary electron yield δ. Typically, the measured sample current of an unbiased sample would be even zero at some energy where $\delta = 1$.) When measuring the current of the biased sample, one would typically run the I_0 measurement before or after acquisition of the LEED $I(V)$ movie, but with the same energy range and steps. Then, the table with the I_0 values (`.csv` or `.tsv` file[2]) should be opened in ImageJ, and this table and the column with the actual beam energies should be selected in *Set Energies, I0, t*. Measuring I_0 before or after the acquisition of the LEED $I(V)$ movie won't help in case of unreproducible jumps of I_0. If this happens, the effect of such jumps can be mitigated by the *Apply fast background changes to I0* option of *Track Spots*.

Footnotes

1 On macOS, you use the ⌘ key instead of CTRL.

2 Comma-separated values or tab-separated values. The decimal separator must be a period, not a comma, and the value separator in `.csv` files must be a comma, not a semicolon.

3 The interpolation utility does no averaging if steps of the input file are closer than the output steps. Thus, if the output steps are too large, information will be lost, leading to an unnecessary increase of the noise.
For a similar reason, the input steps should be at least locally roughly equidistant, otherwise widely-spaced data points get more weight than narrowly spaced points. This would be undesirable when considering noise of the data.

4 Note that the current drawn by the high voltage measurement is typically much higher than the beam current. Thus, when measuring the filament voltage, you cannot measure the beam current I_0 at the same time.